OPERATIONAL SCIAMACHY LEVEL 1B-2 OFF-LINE PROCESSOR:

TOTAL VERTICAL COLUMNS FOR O_3 AND NO_2 AND CLOUD PRODUCTS

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ABSTRACT

The recently updated operational level 1b-2 Off-line data processor for SCIAMACHY (SGP30) contains several updates and evolutions in comparison to the former operational version. The retrieval from nadir measurements in the UV/VIS spectral region had been extended with the cloud algorithm SACURA to obtain the cloud-top height and cloud optical thickness as additional product. The retrieval of total columns for O_3 and NO_2 is now in-line with the scheme applied in the version 4 of the GOME data processor (GDP4). In contrast to GDP4, the cloud-top height and cloud optical thickness from SACURA are used instead of ROCINN. The presentation provides an overview about the evolution of this part of the processor and will close with an outlook to coming versions.

1. INTRODUCTION

Until summer 2006 the off-line processing of Level 2 data products was based on the operational version 2.5 of the SCIAMACHY Level 1b-2 Off-line processor (SGP25). This version contained algorithms for the calculation of the total column density of ozone and NO2 from measurements in the UV and visible spectral region carried in nadir observation geometry, a first algorithm version for the retrieval of ozone and NO_2 profile information from measurements recorded in limb observation geometry, and algorithms for the determination of cloud coverage and the absorbing aerosol index. The determination of total column densities was based on the GOME data processor (GDP) in its version 2.3 and 2.7 which was in between substituted in the operational processing of GOME data by version 3.0 and since the beginning of 2005 by version 4.0. Both versions brought a substantial evolution to the data quality of the GOME total column products. From that, it was decided to transpose the GOME version 4.0 algorithm to the operational processing of SCIAMACHY data and to share the advantage of a similar algorithm baseline for the operational processing of GOME and SCIAMACHY data of total columns. Furthermore, the only cloud product of SGP25, fractional cloud coverage based on OCRA algorithm, had been supplemented by the determination of cloud-top height and cloud optical thickness utilising a sub-set of the SACURA algorithm package developed at the University of Bremen.

For completeness, we note at this point of the paper that the data processor contains also a branch for the derivation of profile information from SCIAMACHY limb measurements in the UV/VIS spectral region. The derivation of ozone and NO_2 profile information had also undergone a full revision with the result that the originally approach was very limited in its potential for further improvements and evolution. Thus, this approach was substituted by the retrieval package DRACULA which was available as in-house development and as a retrieval tool box for *non-linear discrete mathematically ill-posed problems* for SCIAMACHY at DLR. The description of this algorithm update and evaluation is subject to another paper within these proceedings.

The proceeding addresses first for completeness a brief outline of the operational processing chain. After that, the algorithm update for nadir measurements in the UV/VIS spectral region is presented beginning with an overview followed by the cloud and aerosol products and completing with the determination of total column densities of ozone and NO_2. The proceeding is finalized with an outlook to actual developments which are currently under verification for the coming version 3.01 of the data processor. This version is then intended to be the baseline for full-mission re-processing.

2. BRIEF OUTLINE OF OPERATIONAL PROCESSING CHAIN

In Figure 1 we present a sketch of the full processing chain from level 0 to level 2. The details on processing

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of level 0 to level 1b are not subject to this paper. But it should be noted that the operational level 0-1b data processing is carried out in two different modes with the Instrument Processing Facility (IPF) version 6.02: in near-real time mode (NRT) and off-line mode. The main difference between both is the treatment of the calculation of the leakage current which may be a minor source for differences in the determination of column densities in the level 1b to level 2 processing. Operational level 1b to level 2 processing is currently carried out in off-line mode, only. Note that the off-line data processor (SGP25 and SGP30 as well) is total different software as the IPF which contained in former versions (lower than 6) the NRT level 2 processing.

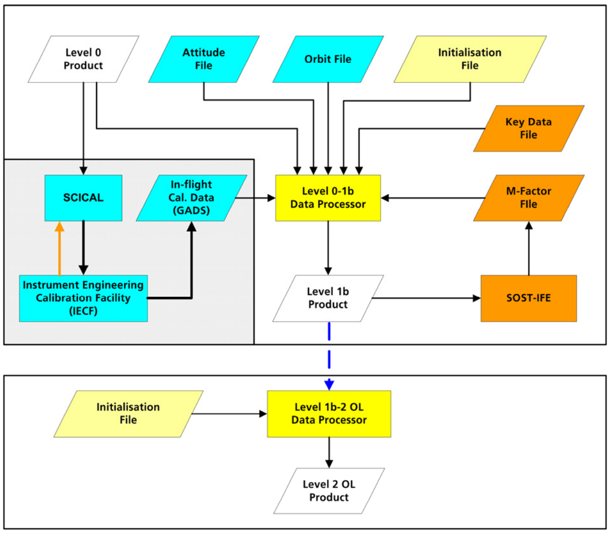

Figure 1. Sketch of the operational level 0 to level 2 processing. Details see text.

Beside the operational processing chain, the data user of level 1b is able to apply the calibration steps individually and optionally with the tool SciaL1c. The results of this tool are calibrated level 1 data which are the called level 1c. Note that in the operational processing the generation and distribution of level 1c products is not foreseen.

3. NADIR UV/VIS ALGORITHM UPDATES

Several products are generated from SCIAMACHY measurement in nadir observation geometry in the UV/VIS spectral region. Those are derived utilising several algorithm steps and different algorithms which can be dependent from each other. Thus, in Figure 2 we show an overview of the algorithm flow in this part of the data processor. The unit "Climatological Pre-processing" combines the processing of all cloud parameters and of the absorbing aerosol index. First, the derivation of cloud coverage from the PMD measurements is initiated utilising the Optical Cloud Recognition Algorithm (OCRA) [1]. The resulting product cloud fraction (CFR) for each spatial pixel based on the shortest integration time of the particular state is provided on one side for the output and additionally as input to the SACURA algorithm [2] for the determination of cloud-top height (CTH) and cloud optical thickness (COT). The result is written into the product, but also provided for the processing of the total column density of ozone and NO_2. For that, cloud-top height is converted to cloud-top pressure (CTP) and cloud optical thickness to cloud-top albedo (CTA). If no result from SACURA is available for the further processing, regress to the ISCCP data base is taken.

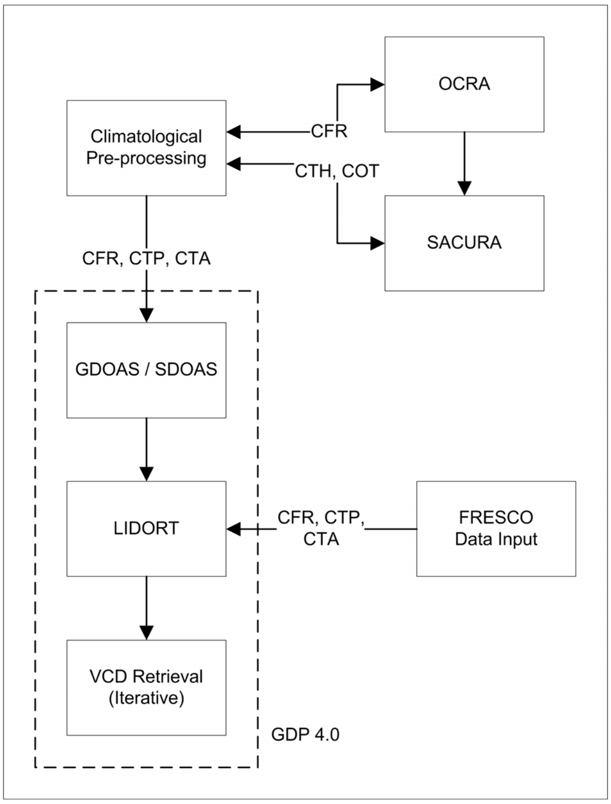

Figure 2. Sketch of the algorithm flow for the nadir UV/VIS algorithms. Details see text.

After the unit "Climatological Pre-processing" a further module is implemented which is mainly based on the GDP 4.0 [3]. This module contains the DOAS implementation as originally developed at the Belgian Institute for Space Aeronomy (BIRA) for GOME (GDOAS) and adapted for SCIAMACHY (SDOAS). The determination of the total column is finally completed by the determination of Air Mass Factors (AMFs) utilizing the Radiative Transfer Model (RTM) LIDORT version 2.2+ and the iterative retrieval scheme for the calculation of vertical column densities. Note that in detail the ozone and NO2 total column derivation differs. For an overview, see below in subsection. A more detailed description can be found in 3.3.

Since the original approach of the total column determination at BIRA is based on cloud products generated with the FRESCO algorithm [4], an instance of the module is available for test and verification purposes. This module instance allows the direct input of the appropriate cloud parameters from file to the determination of the total column density.

3.1. Cloud Parameters and Absorbing Aerosol Index

The implementation of OCRA remained un-changed between version 2.5 and 3.0 of the data processor. The cloud-free reflectance database is based on GOME data; scaling factors which are adapting the storage of the cloud-free reflectance in RGB space to coverage scale from 0 to 100%, had been determined for version 2.5 from SCIAMACHY measurements and are also remained un-changed. Since of these two facts, the cloud fraction can be only an effective one. It is foreseen for further improvements, to recalculate the cloud-free reflectance database from SCIAMACHY PMD measurements and, hence, adjust the scaling factors.

The determination of cloud-top height and cloud optical thickness is a new feature in the operational processing. It is based on a reduced version of University of Bremen's SACURA algorithm which is widely documented (see for example in [2]). The cloud parameters are derived from oxygen A-band measurements. The reduction of the originally retrieval scheme is mainly with the forward modelling which is carried out only once per state since of performance reasons. Internal verifications had shown that this approach is sufficient. Since of the physical model on which SACURA is based, the scheme can be only applied to scenes with cloud fraction higher than 20%. This constraint can lead to a high part of spatial pixel for which then no SACURA results are available for the further processing. In the current processor implementation, a fall-back solution to ISCCP climatology provides then the cloud parameter input to the total column derivation. In order to allow a better data coverage by SACURA, an upgrade of the approach is in final verification for the processing which allows the inclusion of scenes down to cloud coverage of 5%.

The algorithm for the Absorbing Aerosol Index (AAI) remains also unchanged between version 2.5 and 3.0. A cut-off for the solar zenith angle at 80° is contained since the look-up tables for the Rayleigh databases are limited. The AAIA product is written to the Cloud & Aerosol MDS which provides records at each shortest integration time per state. Note that the AAIA is computed at integration time which is mostly longer than the shortest integration time per state so that not all records are filled with information. Unfortunately, the AAIA is currently hampered by the quality of the reflectance of the level 1b product which means a general restriction to the quality of the product. This will also be subject to further algorithm evolution.

3.2. DOAS Algorithm Implementation

The goal of the evolution of the DOAS algorithm implementation is to achieve a substantial improvement for the product quality of the total column of ozone and NO_2. For that, benefit had been taken from the algorithm developments of GDP. Additionally, the compatibility to GDP was one requirement to achieve improvements. Thus, the GDOAS implementation adapted for SCIAMACHY at BIRA, now called SDOAS, had been built up as reference. It is worth to note that no algorithm change between GDOAS and SDOAS must be introduced to transfer the algorithm. The most intense transfer work laid in the determination of correct control parameters of the algorithm, namely the correct usage of reference spectra and wavelength shifts. In case of NO_2, the processing of 60 orbits even distributed over the year 2003 and compared to results of GOME data processing showed that calibration issues interfered in the slant column derivation. Thus, a post-processing for the slant column density had been introduced which is scientifically justified but will be subject to further investigations. Those investigations led again to the recommendation by the validation team to correct the post-processing scheme based on a broader data base. Finally, in the coming upgrade of the processor (version 3.01), the post-processing of the slant column will be removed.

In particular, the derivation of the slant columns for ozone is carried out in the spectral region of 325 to 335 nm. As solar irradiance spectrum the calibrated solar mean reference spectrum measured on the elevation scan mirror (ESM) is in usage. The wavelength calibration of the solar reference is optimized over the fitting interval by taking into account a wavelength shift. This shift had been determined over the fitting interval by means of non-linear least squares on the pre-convolved NEWKPNO atlas. The DOAS algorithm is carried out taking into account the absorption cross-sections of ozone [5] at 223 K and 243 K shifted by + 0.02 nm and scaled by 1.03, the absorption cross-section of NO_2 [5] at 243 K, the Ring effect spectrum convolved of the Kurucz solar atlas with RRS cross-sections of molecular N_2 and O_2, and finally a third-order polynomial. Note that the raw slant column is corrected for the molecular Ring effect as described in [3].

The determination of NO_2 slant columns is performed in the spectral interval of 426.5 to 451.5 nm. The solar irradiance spectrum measured via the azimuth scan mirror (ASM) is taken in un-calibrated mode. As for ozone, the wavelength calibration is extended by a shift

for the solar irradiance. The absorption cross-sections of NO_2 [5] at 243 K, of ozone [5] at 243 K, of O_2-O_2 [6] (with a wavelength axis correction by Burkholder), and of water [7] are applied for the determination of the slant column. Furthermore, the Ring effect is taken during the fit as for ozone, and a polynomial of second order. Finally, the intensities are corrected for an off-set. The result for the slant columns are then corrected by adding an off-set of $+1.0 \times 10^{15}$molecule/cm². This has been justified above.

3.3. Total column density derivation

The total column density derivation is driven by two parts, the AMF calculations utilising the RTM LIDORT version 2.2+ and the determination of the vertical column density (VCD). Note that the scheme to calculate the AMFs are as in GDP version 4.0 including the settings (see []). The AMF calculation for ozone is performed at a wavelength of 325.5 nm in combination with the iterative determination of the VCD. In contrast, the AMF of NO_2 is determined at 440 nm but not in the iterative scheme. In both cases, a geometrical weighting of simple parabolic (1-4-1) is applied for the AMF calculation. The atmospheric climatology in use is the TOMS version 8 ozone profile climatology for ozone and the stratospheric NO_2 climatology of Lambert et al. [3] for the NO_2 retrieval. Temperature profiles are taken from TOMS. Note that the tropospheric NO_2 profile climatology is clean for the NO_2 retrieval. The surface database is based on the GOME LER database [8] and ETOP05 [9]. Finally, the cloud information is prepared by radiance weighting.

The cloud parameters in the operational processing are determined with OCRA (cloud fraction) and SACURA (cloud-top pressure and cloud-top albedo). In case, no data from SACURA are available, values from the ISCCP database are taken. Note that the reference system SDOAS of BIRA makes use of the FRESCO algorithm for the determination of the cloud parameters.

3.4. Verification summary

Since the total column determination of the reference system (SDOAS) is based on the cloud parameter derivation with FRESCO, the verification is performed in two steps. First, reference data had been generated with the original SDOAS algorithm. Those had been provided together with the cloud parameters. These cloud data had then been used in the instance of the processing prototype which allows the input of external cloud parameter. With this verification step a proof of the correct implementation of the total column derivation with respect to the reference could be carried out. The second step contained then the inclusion of the cloud parameters in the retrieval. The results are then compared to the results of the first step. Finally, an inter-comparison to GOME data had been also performed, but this is presented in another contribution of these proceedings. Note that the verification test database consists of 60 orbits of 2003 even distributed over all seasons.

We can summarize the results of the first step (SDOAS original versus processor prototype instance in combination with FRESCO cloud data) as follows: One observes for the ozone VCDs a mean deviation of around -0.4% with a standard deviation of 0.35%. 97% of the test data match the 1% level. The differences between processor implementation and reference are easily explained (and verified). The climatological databases are extracted by nearest neighbour in season and geo-location for the reference system. In contrast the extraction of climatological databases in the operational processor is carried out utilising interpolation schemes for seasons and geo-location. In case of NO_2, the mean deviation is also around -0.4% with a standard deviation of 0.25%. Here, we can observe that most of the data match the 1% level.
The second verification step, i.e. the inter-comparison of the same retrieval scheme but based on the different cloud parameter input, can be summarized to: the mean deviation of ozone VCDs is around +0.4% with a standard deviation of 1.4%. In case of NO_2 VCDs, a mean deviation of around +0.02% with a standard deviation of around 0.25% is observed. It is not surprising that the deviations in case of NO_2 are smaller since the VCD retrieval is based on an atmospheric climatology with a clean troposphere.

In order to avoid a misinterpretation of the product results, we like to point out that the slant column density results are provided in the product of version 3.00 without the Molecular Ring correction. Additionally, the operational level 2 product is based on the level 1b product which is computed in off-line mode. In general, the difference for ozone total columns is less than 0.01% but one can observe some cases where the difference is around 1% and higher. In case of NO_2 the difference between usage level 1b NRT and level 1b offline product is more pronounced and can vary around 1-4%.

4. FURTHER DEVELOPMENTS AND OUTLOOK

The update of the operational Level 1b-2 off-line data processor introduced a substantial improvement for all total column and profile products. However, the cloud and aerosol products are subject to further evolutions in the near future. Currently, an update of the processor to version 3.01 is under verification. This update contains an update of the SACURA algorithm which allows the determination of cloud-top height and cloud optical

thickness for cloudy scenes down to coverage of 5 %. Furthermore, the fall-back to ISCCP will be switched off.

Further evolutions to the total column and profile products are planned and envisaged in the context of the SCIAMACHY Quality Working Group for later updates. There are also intentions to bring new products in the pipeline, especially a first operational product from SCIAMACHY infrared measurements. Note that an ambitious update cycle of the processor is planned and a major update after the update to version 3.01 can be expected beginning of next year.

5. REFERENCES

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